## 2000-499800/45

A25 D21 E19 G02 (A12 A41 G03 G05) BADI 1998.12.23

BASF AG

\*DE 19860041-A1

1933.12.23 1998-1060041(+1998DE-1060041) (2000.06.29) C07C 265/14, A61K 6/08, C07C 275/60, C08L 75/04, C09D 175/04

New low-viscosity, radiation-curable isocyanate compounds dualcure coating systems, contain activated carbon-carbon double bonds

C2000-150124

Addnl. Data: BRUCHMANN B, BECK E, RENZ H, KOENIGER R, SCHWALM R, LOKAI M, REICH W

**NOVELTY** 

Novel compounds (I) have isocyanate or capped isocyanate groups, allophanate groups and radically polymerizable C-C double bonds activated by a directly bonded carbonyl or group or by an O-atom in an ether function. (I) are derived from polyisocyanates and alcohols (A) containing the activated double bond (as well as the OH function).

DETAILED DESCRIPTION

INDEPENDENT CLAIMS are included for:

(a) mixtures containing:

A(5-F1E, 5-G1E, 5-J, 5-J1A, 5-J2, 5-J4, 8-C7, 8-C9, 11- 
A2, 11-B5, 11-C2B, 12-B1K) D(8-A5) E(10-A12C1, 10-A12C2, 10-A13B1, 10-A13B2) G(2-A2B2, 2-A2H, 2-A4A, 2-A5, 3-B2E, 3-B2E4, 5-A)

(i) 1-100 wt. % (I); and

(ii) 0-99 wt. % of a compound containing at least one NCO group plus a group selected from urethane, urea, biuret, allophanate, carbodiimide, uretonimine, uretdione and isocyanurate;

(b) preparations containing:

(i) 1-99 wt. % (I) or mixture (a); and

(ii) 99-1 wt. % of a compound (other than (I)) having at least one radically polymerizable double bond:

(c) 2-component coating compositions comprising (I) or mixture (a) plus compounds containing groups reactive with NCO groups, the ratio of NCO groups to NCO-reactive groups being 0.5-2:1;

(d) the preparation of (I);

(e) methods for coating articles using (I) or (a)-(c), involving:

(1) applying the materials and either:

 (i) optionally pre-hardening by polyaddition reaction of the NCO groups; and

(ii) irradiating with high-energy radiation, or heating at temperatures

DE 19860041-A+

up to 130 °C;

(2) applying one of the following:

(i) applying a coating of the materials;

(ii) prehardening with high energy radiation;

(iii) mechanically processing (specifically shaping) the article or contacting with other articles; and

(iv) hardening by NCO polyaddition reaction; or

(3) as in (2) except that step (ii) is effected by NCO addition reaction and step (iv) by irradiation, and

(f) articles coated by the methods (e).

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The coatings may be applied to e.g. wood, paper, textile, leather, non-woven, plastics, glass, ceramic, mineral or especially metal substrates. In addition to coatings, (I), mixtures (a) and preparations (b) are used in casting resins, filler compositions, stereolithography resins, printing plates, printing inks, adhesives or dental compositions or as resins in composites (all claimed).

**ADVANTAGE** 

The (I)-based coating systems have low viscosity (e.g. 100-30000 mPas at 23 °C) at minimal solvent content, and are easily processed

and handled. They can be used as 'dual-cure' systems, where the prehardened coatings are non-sticky, flexible and elastic so that the articles are readily transported and further processed before final hardening (e.g. by chemical methods in the absence of irradiation). Hardening by irradiation takes place quantitatively at low doses of radiation.

**EXAMPLE** 

A mixture of hexamethylene diisocyanate (HDI) and hydroxyethyl acrylate (5 mol. % based on HDI) was heated to 80 °C, treated with 200 ppm (based on HDI) of N,N,N-trimethyl-N-(2-hydroxypropyl)-ammonium 2-ethylhexanoate (catalyst), heated slowly to 120 °C, reacted until the NCO content of the mixture reached 40.8 wt. %, quenched by adding 250 ppm (based on HDI) of di-2-ethylhexyl phosphate and evaporated at 135 °C/2.5 mbar to remove unreacted HDI. The NCO content after distillation was 20.1 wt. % and the viscosity was 520 mPas at 23 °C. The obtained polyisocyanato-acrylate (containing urethane and allophanate groups) was mixed with Lumitol H136 (TM) (RTM: hydroxy-functional vinyl polymer) at a stoichiometric OH/NCO ratio. The obtained clear lacquer was coated on a glass plate at a wet thickness of 200 µm,

DE 19860041-A+/1

## 2000-499800/45

prehardened under ambient conditions and hardened by irradiation with a high pressure mercury lamp (20 W/cm).

## **TECHNOLOGY FOCUS**

Organic Chemistry - Preferred Compounds: (I) are of formula (I');

$$0 > N - R_1 - R_2 - R_1 - N > 0$$
 (I')

n = 1-10;

R<sub>1</sub> = 2-20C aliphatic or alicyclic hydrocarbylene or 5-20C aromatic hydrocarbylene;

one  $R_2$  in each repeating unit = NH and the other = N-C(O)- $R_3$ ;  $R_3$  = residue of (A).

Alcohol (A) specifically an ester of an aliphatic or aromatic polyol or an aminoalcohol with (meth)acrylic acid; or vinyl ether derived from an aliphatic or aromatic polyol. The polyol is preferably a 2-20C di-, tri- or tetrol, a polyether or polyester polyol or a polyacrylate-polyol of average OH functionality 2-10. R<sub>3</sub> is especially derived from hydroxyethyl (meth)acrylate, hydroxypropyl acrylate, hydroxybutyl acrylate or 3-(acryloyloxy)-2-hydroxypropyl methacrylate. The isocyanate component is hexamethylene diisocyanate, isophorone diisocyanate, tetramethylxylylene diisocyanate, di-(isocyanatocyclohexyl)-methane or 1,3-bis-(isocyanatomethyl)-

(isocyanatocyclohexyl)-methane or 1,3-bis-(isocyanatomethyl) cyclohexane.

Preferred Preparation: Claimed preparation of (I) involves reacting a diisocyanate with the alcohol (A) at 80-280 °C.

Polymers - Preferred Compositions: Mixtures (a) contain 0.02-20 wt. % activated double bonds and 0.1-40 wt. % isocyanate groups, and have a ratio of activated double bonds to isocyanate groups or 50: 1 to 0.02: 1.

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DE 19860041-A/2